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Experiences Gained in System Design, Development, and Implementation of an Automated, Computer-Based, Water Quality Analytical Laboratory Data Capture/Management System

G.S. Beal,* F.J. Philbert† and J.E. Dowell*

*National Water Research Institute
Inland Waters/Lands Directorate
Canada Centre for Inland Waters
Burlington, Ontario

†Water Quality Branch
Inland Waters/Lands Directorate
Ontario Region
Burlington, Ontario

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Contents

	Page
ABSTRACT	v
RÉSUMÉ	v
INTRODUCTION	1
HISTORICAL BACKGROUND	1
SYSTEM CONCEPT AND DESIGN	2
SYSTEM SPECIAL HARDWARE	5
SOFTWARE	8
THE FINAL SOLUTION	9
CONCLUSION	9
ACKNOWLEDGMENTS	9
REFERENCES	10

Tables

1. List of instruments identified in the system functional requirements document to be interfaced to the computer	3
2. Nature and frequency of reports to be generated (as listed in the system functional requirements document)	4

Illustration

Figure 1. AWQUALABS block diagram	6

Abstract

There are specific logical steps to be followed when designing, developing and implementing an automated computerized system for an analytical laboratory. Any significant deviation from the recommended procedure could potentially impede progress or lead to failure in achieving the goals set for the project.

AWQUALABS is a computer-based **A**utomated **W**ater **Q**uality **A**nalytical **L**aboratory **S**ystem. The AWQUALABS development team, charged with the task of designing and developing an automated computerized system for the Water Quality Branch laboratory of Environment Canada, had major constraints imposed upon it from the system's inception. We recount in this report how we proceeded with the design and development of the system, some of the problems we encountered, and how we eventually managed to resolve them.

Résumé

Certaines étapes logiques doivent être respectées dans la conception, l'élaboration et la mise en application d'un système informatisé pour un laboratoire d'analyse. Tout écart sensible par rapport à la procédure recommandée peut nuire à l'avancement du projet ou empêcher celui-ci d'atteindre ses objectifs.

AWQUALABS est un système informatisé du laboratoire d'analyse de la qualité de l'eau. L'équipe qui a été chargée de concevoir et d'élaborer AWQUALABS pour le laboratoire de la Direction de la qualité des eaux d'Environnement Canada s'est vu imposer des contraintes majeures dès le départ. Nous racontons dans ce rapport comment nous avons procédé pour concevoir le système et le mettre au point, ainsi que la façon dont nous avons résolu certains des problèmes rencontrés.

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INTRODUCTION

There is a natural order to most processes and, if at all possible, one should enforce its preservation. The natural order for the design and development of a computer-based system is first to decide on all the application details, such as data volumes, throughputs and computations, and secondly, to select a suitable hardware configuration. At the beginning of the project, an implementation team should be assembled to determine specific pieces of hardware and software for the job.

The following is an account of our experiences in designing, developing and implementing an automated computerized water quality analytical laboratory data capture/management system (AWQUALABS) in Environment Canada's Water Quality Branch Analytical Chemistry Laboratory at Burlington, Ontario. We believe that this report should be of interest and benefit to others involved in the computerization of laboratory operations. A description of the system itself can be found in Inland Waters/Lands Directorate Technical Bulletin No. 149 (Philbert *et al.*, 1987).

HISTORICAL BACKGROUND

Through the initiative of the Laboratory Operations Division, Water Quality Branch (WQB), Headquarters, a feasibility study was undertaken by Digital Methods Ltd. (DML) and a report was produced in 1974. The report indicated that it would be cost-effective to computerize operations in the WQB regional laboratories and it recommended that the first system be developed in the Ontario Regional lab at Burlington (Digital Methods Ltd., 1974). The DML feasibility study report was followed about one year later by the acceptance of an unsolicited proposal by DML, resulting in the production of a preliminary data capture and management system together with a five-volume report detailing a perceived system (Digital Methods Ltd., 1975). DML demonstrated the system at the Ontario Region lab in 1976 as part of the contract. It was noted in the demonstration report that the purpose of the demonstration was to show the capability of developed algorithms, but that the software system, as configured, was not intended for operational use (Digital Methods Ltd., 1976). Immediately thereafter, another report detailing the functional specifications for a computerized laboratory system in the Ontario lab was prepared by A. Demayo (1976) under contract to the Department of Fisheries and Environment.

Because additional funds were not available to continue the development by contract, the decision was made to utilize in-house expertise to develop the laboratory data system. A study team, comprising personnel from the Water Quality Branch, and the Electronics Engineering and Data Management sections of the National Water Research Institute (NWRI), was formed in February 1977. The development of what was to be the first system of its scale in Environment Canada commenced three months later with the first meeting of the study team in April.

The study team was charged with developing a pilot system in two phases. In Phase I, a data capture system that would be capable of real-time capture, preprocessing and analysis of raw data for the WQB laboratories was to be developed within one year. A Digital Equipment Company (DEC) PDP 11/34 computer with 32K words of memory, two 1.2M word disk drives and the RT-11 operating system was provided for this purpose. Apart from a manual entry facility, the system was to have two atomic absorption spectrophotometers, two three-channel Technicon Auto-Analyzers®, one gas chromatograph/Spectra Physics-4000 (GC/SP-4000) system, one Hewlett-Packard CHN Analyzer, and one total/dissolved organic carbon analyzer on line by the end of Phase I. Phase II of the project was to encompass data management functions including the organization, management and reporting of analytical results generated by the laboratory. The developed system was to be amenable to future expansion and modification, as required, and transferable to four other WQB regional laboratories across Canada, some of which already had PDP-11 series computers.

The budget estimated for the first year of the project amounted to $30 000 capital, $4500 operating and maintenance, and 2.96 person-years of programmers and systems analysts time ($53 000 salary). This can be compared with the total cost for the development of the system, which is estimated to be $1.2 million. This figure includes costs of all related activities including system maintenance, system enhancement, modifications and evaluation, bench-marking of the VAX computer, user training, and salaries for a system manager throughout.

The need for a more detailed and specific set of functional requirements than those originally available was established within three months of the first meeting of the development team. Thereupon, the first major undertaking by the team was to prepare a suitable functional requirements document (Beal *et al.*, 1977) in accordance with the ASTM Committee E31 Guidelines on Computerized Laboratory Systems.

The PDP 11/34 computer was replaced in March 1978 by a Digital PDP 11/60 machine on which the AWQUALABS system of programs was developed using RSX-11M, BASIC Plus 2 and RMS-11K.

The first real sample analysis report was produced on the system for formal submission in November 1979. The first phase of program development was completed in October 1980. The evaluation of the system under real conditions was scheduled for completion by March 1981. However, further requests by laboratory personnel for enhancements, coupled with computer-related problems, delayed the process. Ongoing evaluation of AWQUALABS, along with bench-marking exercises on a VAX 11/750 system (courtesy of Digital Equipment Corporation), led to the replacement of the PDP 11/60 computer with a VAX 11/750 machine in March 1983. System performance was then improved by a factor of at least ten times and user confidence and satisfaction were restored as a result of the progression to a more powerful computer.

SYSTEM CONCEPT AND DESIGN

The initial hardware configuration presented to the implementation team was a Digital Equipment Corporation (DEC) PDP 11/34 minicomputer with two RK-05 disk drives (2.5 million bytes of data each) and 32K words of main memory. The software available was RT-11, FORTRAN and Interactive BASIC. This was an upgraded system from the one provided to Digital Methods Ltd. for their feasibility demonstration of the data capture and reporting system for gas chromatographs and autoanalyzers, and included the Industrial Control System (ICS-11) interface. The acquisition of hardware before the application needs had been established placed a number of serious constraints on the development team.

The development team drew up rough design criteria and decided that with the small amount of money available, the system could be expanded to include eight terminal lines and a line printer. The plan was to mechanize the data acquisition and computations from two Perkin-Elmer model 403 atomic absorption spectrophotometers (AAs) and some Technicon AutoAnalyzers (TAAs). Work began on some simple data acquisition software to run under RT-11. A simple box was designed for the AAs comprising a universal asynchronous receiver-transmitter (UART) and power supply. The device accepted the byte-parallel output from the printer port and sent it bit-serial to the computer.

As we proceeded, however, we decided that a complete data management and reporting system, as well as connection of as many of the laboratory instruments as possible to the computer, would be more advantageous than the scheme originally requested by management. Therefore, all current aspects of lab operations were evaluated and examined for inclusion in the system. All reports, calculations and quality control considerations were included as well as all temporal variables, including turnaround requirements. Thus, the system functional requirements document by Beal *et al.* (1977) reflected a major increase in the scope of the project in that it now represented an effort to computerize completely all practical aspects of the laboratory operation. As shown in Table 1, most of the instruments to be interfaced were located on the 7th floor of the laboratory building with a few others on the 5th floor. The specifications on reports to be generated are listed in Table 2.

Simple calculations based on the number of samples processed each year and the projected turnaround time for the results gave a figure of the amount of disk storage required to hold these intermediate results as well as an idea of the processing power required. It was about an order of magnitude larger than the configuration at that time.

Another disquieting aspect was the requirement that many of the instruments be run simultaneously and that the actual mix would be variable. This led to a decision to upgrade the PDP 11/34 to include larger disks, more memory, and additional communication lines. An obvious upgrade to the software was also required because the RT-11, at that time, could not handle more than 28K words of main memory. A multi-user system was required.

One aspect of analytical instrumentation was becoming commonplace. Manufacturers were including mini- and even microcomputers in their instruments. Therefore, most had some type of interface for "Teletype-like" printers.

This proved to be a great blessing for the integration of the instruments with the AWQUALABS computer system. The data produced by the instrument could be entered directly into the system, since the instrument appeared to the computer as a user typing at a terminal. The analog observations were reduced to ASC II characters at the instruments, so that when sent to the AWQUALABS system, some of the computational load was removed. Thus, instrument interfaces were largely simplified into terminal lines.

Initially, the intended approach has been to develop the requisite software from scratch while making use of the software already developed by DML and the WQB Atlantic Regional Laboratory. However, the high cost estimated for in-house software development led to a search for a better and more cost-effective way to develop the system. Much valuable information was acquired by contacting or visiting several people and institutions in Canada and the United States, and some in England. At the same time, the team investigated other computer systems, including those by

Table 1. List of Instruments Identified in the System Functional Requirements Document to Be Interfaced to the Computer

Type	Make	Model	Location	Qty.	Interface type	Comments
Atomic absorption spectrophotometer	Perkin-Elmer	603	L736/L738	1	SD	
Atomic absorption spectrophotometer	Perkin-Elmer	403	L736/L738	3	SD	Three channels
AutoAnalyzer	Technicon	II	L761	2	SD	Two in Phase I
Gas chromatograph processor	Spectra-Physics	4000	L771	1	SD	Handles 11 GCs
CHN Analyzer	Hewlett-Packard	185B	L761	1	N/A	Output will be entered manually
Automated carbon analyzer	Technicon/Beckman	315/865	L761	1	Analog	Two channels
UV spectrophotometer			L510	1	SD	
AutoAnalyzer	Technicon	II	L761	3	SD	Two channels
CHN Analyzer	Hewlett-Packard	185A	L761	1	Analog	Two channels
AutoAnalyzer	Technicon	II	L510	1	Analog	One channel
Atomic absorption spectrophotometer	Perkin-Elmer	403	L510	1	SD	
Total alkalinity	Beckman	865	L745	1	Analog	
AutoAnalyzer	Technicon	II	L745	1	SD	Three channels
AutoAnalyzer	Technicon	I	L745	1	Analog	Two channels of CSM-6
Emission spectroscopic system			L747 (tentative)	1	SD	
Mass spectrometer	Finnigan		L768	1	SD	
Automated Hg analyzer	Technicon/?		L510	1	Analog	One channel
Automated Cn analyzer	Technicon		L730	1	Analog	One channel
New and/or additional instruments as they become available						

SD – Serial-digital.

Hewlett-Packard and Data General, in an attempt to take full advantage of the then current state of the art in striving for an optimal solution. After reviewing the available options and their respective costs and flexibilities, we decided to use the available PDP 11/34 machine, upgraded by add-ons, but now using the RSX-11M operating system and RMS-11K.

Shortly thereafter, the DEC salesman presented another option. We could upgrade the entire computer on a "trade-in" basis to the newly announced PDP-11/60, a more powerful computer with 64K words of memory and two RKO6 disk drives, giving a total of 32 Megabytes of storage. The operating system was to be upgraded from RT-11 to the new, multi-tasking RSX-11M at the same time. In addition, a data manipulation tool called "Datatrieve" became available, and results of preliminary investigations by the AWQUALABS development team members were positive. The package would be a useful addition during the development of the software, since preliminary reports and database searches could be conducted easily; once the design of the reports and the scheme of the searches had

Table 2. Nature and Frequency of Reports to Be Generated (as listed in the system functional requirements document)

Name	Medium	Size	Frequency	Delay	No. of copies
Run report	LP	1-2 pp.	35/day	5 min	1
Preliminary sample analysis report	LP	1-2 pp.	50/week	5 min	As requested
Final sample analysis report	LP	1-2 pp.	20/week	12 h	As requested
Containers in process report					
- summary	TT	2-20 lines	20/day	10 s	N/A
- listing	LP	1-2 pp.	20/week	10 min	As requested
- matrix	LP	1-2 pp.	20/week	10 min	As requested
Samples in process report					
- summary	TT	4-20 lines	20/week	10 s	N/A
- matrix	LP	5-10 pp.	20/week	1 h	As requested
Samples completed report	LP	2 pp.	5/week	1 h	1
Laboratory workload report	LP	8 pp.	1/month	12 h	As requested
Operational performance measurement system (OPMS) indices	LP	2 pp.	2/week	1 h	1
NAQUADAT tape	9-track mag tape	N/A	1-5 weeks on demand	7 days	1
STAR tape	9-track mag tape	N/A	1-5 weeks on demand	7 days	1
Resource usage report					
- study/project	LP	2 pp.	≥1/ month	12 h	1
- agency	LP	1 p.	≥1/month	12 h	1
Quality control checks report	LP	2-10 pp.	3/week	12 h	3
Study/project listings and Summary report	LP	6-10 pp.	5/week	10 min	As requested
Study/project description report	LP	1 p.	120/yr	12 h	≤4
Assignment record	LP	5-10 pp.	3/day	12 h	1
Sample container control report	LP	5 pp.	1/day	12 h	1
SP4000 Interim report	TT	6 lines	3/day	10 s	N/A

LP – Line printer.
TT – Teletype.

been chosen, they could be re-coded into specific programs. Also, "one-of-a-kind" reports could be generated easily, and file maintenance, where small yet significant problems were involved, would be made simpler.

Datatrieve, as it turned out, was not as useful as had been anticipated. The data structures in AWQUALABS were far too complex to define to the version we had initially received (although it is now quite suitable), and the memory required to run it imposed a severe penalty.

Since it would take some time to acquire the PDP 11/60, arrangements were made to pre-deliver the software. Before the arrival of the hardware, work progressed using the new RSX-11M, BASIC and RMS-11K software on the existing PDP 11/34. Because the software was compatible among the machines used, little disruption to development was experienced. This feature permitted us to change the system later with little impact on the users.

One decision made by the team at this point had both positive and negative aspects, which were later determined during a review of the project. We decided that all software for the project should be written in a common high-level language. This meant that the system would be portable to other computers, with minimum disruption and re-development, should a further increase in capabilities be required. From this perspective, the decision was sound. However, the selection of the BASIC language for implementation later proved questionable. The choice at the time seemed wise, considering that (1) BASIC was available on most machines in the marketplace; (2) the data management system available for the PDP-11 was RMS-11K, an indexed-sequential system with significant capabilities and with BASIC being the only high-level interfacing language; and (3) Datatrieve also required the use of RMS-11K.

In retrospect, BASIC was not a uniform language among its various implementations, and our desire to use RMS-11K for the storage organizer led us to use DEC extensions to the language which would have been impossible to transport to other vendors' machines. One positive aspect about the BASIC implementation was that it used a compiled version and the code ran reasonably quickly. On the other hand, the size of the modules created, owing to the attachment of the RMS-11K library, had a negative effect on system performance (sharable libraries were not yet available for RMS-11K). The excessive size of the programs meant that no more than one could be run at a time without substantial executive time being consumed in swapping the competing tasks.

DEC eventually acknowledged that 64K words was too little for our requirements, in spite of having been asked, prior to our procurement of the machine, to specify and supply the configuration required to meet the functional specifications. Thus, another 64K word module had to be acquired. The resulting difference in system performance was like night and day. The nightmare performance of the small memory was replaced by daydreams of new and wonderful features.

Although the most logical decisions were made at the time, in retrospect perhaps the language "C" would have been a better choice. We would have had to write our own data storage system but would have gained in areas of storage efficiency and performance. We would not have had to cope with the excessive overhead of RMS-11K in BASIC because we would have written proper interfaces for "C".

SYSTEM SPECIAL HARDWARE

As noted in the AWQUALABS Special Hardware Handbook Notes (Harrison, 1982), the primary concerns in the design of the AWQUALABS hardware system were to make as much use of the standard hardware and interfaces as possible, and to simplify the overall architecture of the system. The decision was made to use primarily serial-digital data transmission in the system, since most of the instruments were readily adaptable to this technique by means of procurable interfaces. The system hardware block diagram, as it then related to the system, is shown in Figure 1. It provides a functional overview of the system at its initial stage. As mentioned above, organizational changes have since resulted in a number of major modifications to the layout.

All "work stations" were to be provided with two links to the computer: one for the instrument and one for the analyst's terminal. "Blue boxes" were placed in most of the labs and cable was laid in the troughs. The terminations of these cables in the computer room were in a separate rack with a patch panel to allow for reconfiguration of the lines. The termination panels for the DX-11 communication interfaces were mounted in the rack, as was the ICS-11 subsystem. The ease of access to this rack made testing and re-wiring simple.

All communication in the system was by four-wire, 20-milliamp current loop with the instrument being passive. The reason for this was the RS-232C 25-foot limit on the distance for EIA connections. As the distances within the lab were much larger than this limit, current loop interfaces, which do not suffer the same distance limitation, were installed. An off-the-shelf Belden cable was ideal for the connections. It offered two individually shielded quads

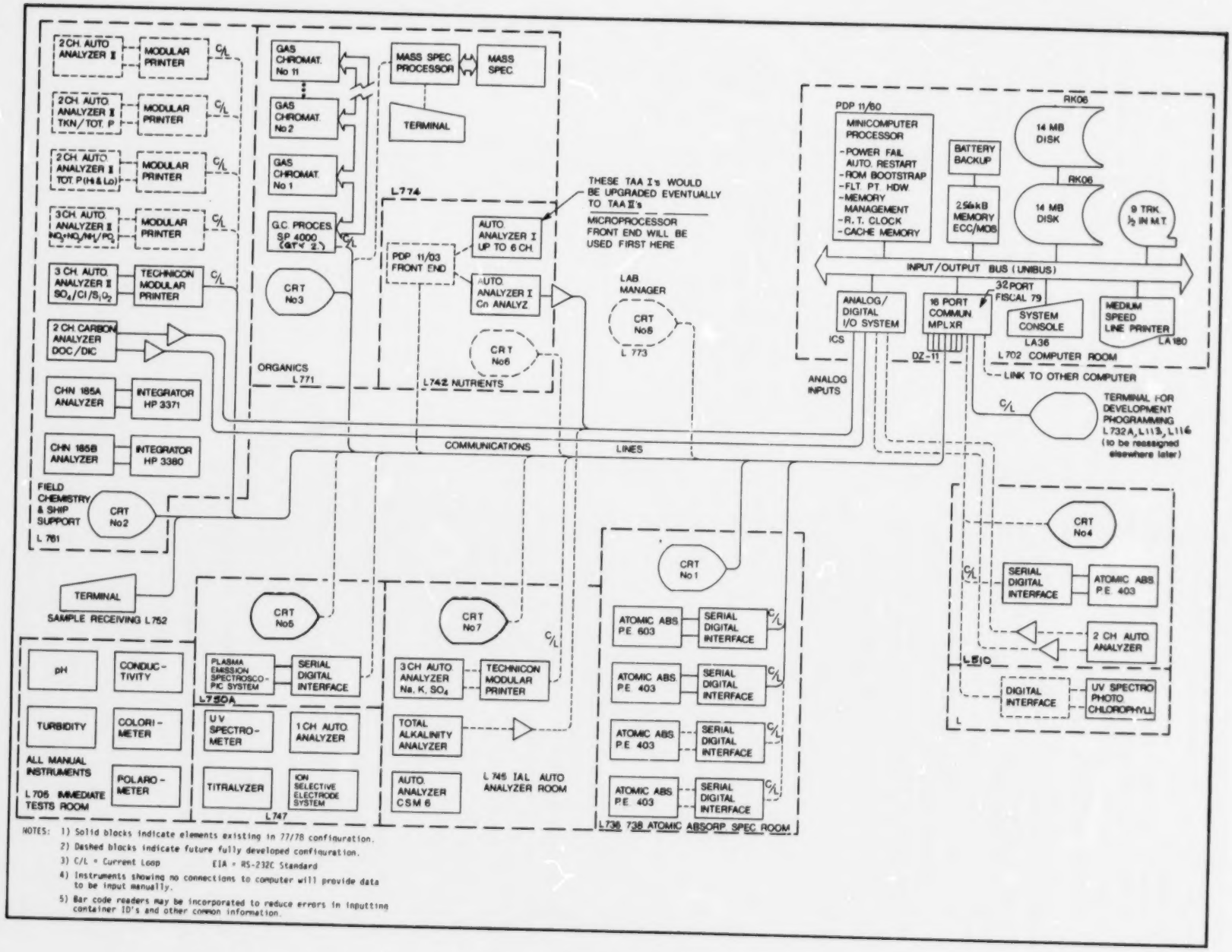

Figure 1. AWQUALABS block diagram.

and an unshielded pair in a vinyl jacket. One quad could be used for the instrument, the other for the user terminal, and the unshielded pair for an intercom back to the computer room to facilitate testing. Some 1800 m of this cable was run on the 5th and 7th floors of the building.

Once the current loop interface had been selected, terminals were required. The team selected Hazeltine model 1500 terminals, since they were the least expensive, offered a current loop interface usable to 19 200 baud, and had a numeric keypad for data entry. All terminals in the lab were to be the same to minimize the trauma that could be caused by moving to a keyboard with a different layout.

A suggestion to use bar code readers to input sample identification information to the computer was investigated. Under this scheme, coded identification labels were to be fixed to each sample container and bar code readers connected to each terminal. The user could use the wand to read the sample number and thus eliminate typing errors. Furthermore, sheets of coded information could be produced which contained text otherwise requiring repetitive and error-prone typing (program run instructions, parameter names, etc.). Ten bar code readers were purchased and interfaced to terminals. Although the concept was basically sound, the developmental aspects of the project meant that sample number formats and program typeins changed frequently, and the use of bar code readers was therefore discontinued. Moreover, the use of an "auto increment" entry program which automatically initialized samples sequentially proved to be a satisfactory solution. At this point in the development, the hardware configuration became more or less fixed. It was acknowledged that new instruments would be added and obsolete ones deleted. The decision to interface everything by means of communication lines permitted wide varieties of devices to be connected without difficulty. All that was necessary was to write a new, or modify an existing program to receive the data, which proved fairly easy.

There have been numerous changes made in both laboratory instrument types and their location over the course of AWQUALABS development. For example, most of the modular printers for the Technicon AutoAnalyzers have been replaced with data systems from Pulsar Electronics. These boxes do the peak detection, standards calibration and data communications for up to three channels and have proven to be more reliable than the Technicon devices, which used mercury-wetted relays for 110-baud terminal communication. Although we found program modification relatively simple to perform to accommodate this new device, we experienced some difficulty in down-loading the analyst's tray patterns to the device. We decided to use a method by which the sample number was set to its position number and then let the AWQUALABS computer keep the relationship straight. A special-purpose program, named PULSAR, was developed which was capable of down-loading sample information into the PULSAR unit, and up-loading the results from the original sample set after the analysis was complete. Once communications between the VAX and the Pulsar device had been successfully established, the utility was completed and put into production in a relatively short time.

The advancement of the implementation phase of AWQUALABS immediately identified a need for an improved method of handling information from samples analyzed aboard ship. Shipboard analysis of some chemical constituents was traditionally done with Technicon AutoAnalyzers equipped with automatic printers (Philbert *et al.*, 1976). The analytical results were then manually processed and transcribed onto a variety of report forms or entered into the computer using a terminal.

The process was automated by means of a Hewlett-Packard 85 microcomputer (HP-85) system. The resultant shipboard data acquisition system (SDAS) is portable, and collects, stores or reports on a built-in printer the analytical results along with the associated ancillary information. The system is menu-driven and automatically updates predictable information such as sequential sample and station numbers. The analytical results and related information are collected and stored on cassette tape. At the end of each survey, the SDAS calculator is returned to the main laboratory and connected to the AWQUALABS computer for direct sample initialization and data submission. The SDAS automatically logs onto the AWQUALABS computer, creates files, transfers the data and runs a program to initialize the samples and update the database.

The program that permitted the HP-85 system to talk to the database was implemented easily and provides an error-free method of storing and transferring the data. A diagrammatic representation and specifications of the system are available elsewhere (Ford, 1984).

In 1979, the laboratory acquired an Applied Research Laboratories (ARL) inductively coupled argon plasma spectrometer system (ICAP) equipped with a DEC PDP 11/04 computer. After some work by ARL, the system was able to produce the reports required by the lab. ARL also produced software to enable the data system to communicate with the AWQUALABS software. Unfortunately, the specification for the communications scheme desired (the PULSAR "echo checking" protocol) was not provided to ARL. As a result, the protocol chosen by ARL in the software they provided proved to be difficult to use with the BASIC on the VAX computer. Consequently, some

external consultants familiar with the VAX and the VMS operating system were contracted to examine the problem and provide a solution. This task included also the software interfacing of another ARL ICAP device acquired in 1985.

The consultants identified and resolved a number of data communication problems during this exercise:

(i) The ICAP devices failed to recognize X-on/X-off when communicating with the VAX. The VAX was accordingly adjusted to accommodate this.

(ii) The ICAP devices are highly unlikely ever to transmit a packet of data in excess of 1000 bytes. Adjusting the size of type-ahead buffers for terminal devices on the VAX from 256 to 1024 bytes was sufficient to ensure data would not be lost.

(iii) The older ICAP failed to receive the appropriate handshaking signals, as it was reading in the next data record to be processed when it should have been handling the data communication responsibilities first. This problem was overcome by throwing a delay factor into the ICAP utility when conversing with the older device. This delay factor is automatically disabled when the ICAP utility detects that it is in communication with the newer ICAP.

(iv) Although the manufacturer's documentation had indicated that the check-sum calculations for both the old and new ICAP devices were identical, it was discovered that this was not the case. The older ICAP device was modified to produce check-sum calculations identical with those of the newer instrument.

The consultants produced a DCL (Digital Command Language) command-based utility capable of retrieving data from both ICAP devices, which places the information directly into tray pattern files ready for processing by AWQUALABS. The utility provides the user with great flexibility. The analyst can selectively disregard or update information sent from the ICAP devices. The analyst need not be concerned with the location of information in the tray pattern files, as the utility assumes all responsibility for correct positioning of data within the tray pattern files. The utility does not even require pre-defined tray pattern files, since it is capable of creating tray pattern files as needed.

SOFTWARE

Because AWQUALABS was required to handle many different tasks at once, including data acquisition, report generation and database updates, the multi-tasking features of RSX-11M were very useful. We could assign priorities to tasks so that the data acquisition functions would not be hindered by the more mundane and less time-critical tasks of database operation. Or so we thought. . . It turned out that system thrashing on RMS-11K tasks had a negative impact on real-time performance. Various schemes were tried to circumvent this, but the problems were deep-seated. In the end, we limited certain tasks to run only at night. Problems were encountered when program development was attempted simultaneously with lab operations, so that eventually we had to schedule work among the lab personnel and program developers. This proved awkward but, unfortunately, necessary. Shortly after these problems became apparent, a new release of RSX-11M eliminated many of the difficulties we had encountered. However, because the executive portion of 11M had grown, we now had less address space available for user tasks. We could remain with the older version of 11M with its attendant problems of scheduling or rewrite many of our programs to fit the new version and thus have better scheduling. We elected to do the latter and found the performance improved when the machine was running. However, we began having trouble with system crashes. Arbitrarily, it seemed, the system would just fail; the only discernible cause was loading, so once again we were forced to limit operation on the machine for particular tasks to certain times of the day.

This unsatisfactory situation eventually eased after new releases of the 11M software became available to fix internal troubles with the operating system. Nevertheless, the promised improvements in operation had not materialized, and the analysts found it easier to work in the old way, with pencil and paper.

After the internal problems were treated, or accommodated, work progressed on the software. User feedback on our implementations led to rewriting of some tasks and extending others. New tasks were written and tried, and additional user feedback was always forthcoming. The system was developing functionality and utility to the user community.

With the basic structure of the system laid out and the application tasks taking shape quickly with the required functionality, users began to rebuild the confidence so quickly eroded when the system was not operating properly. But even with renewed interest by the analysts, there was still one nagging problem, i.e., the aggregate performance of the machine was inadequate as far as complete lab operations were concerned. The system was still rationed to certain tasks at specific times of the day. Although the lab personnel could adapt to the schedule, the arrangement was clearly unsatisfactory.

THE FINAL SOLUTION

The analysis of the system performance problem pointed to one simple fact. There was a lot of disk activity involved in searching the various threads of data in the files collectively known as "the database." Proposed solutions, based upon upgrading to larger PDP-11 systems, all had the same Achilles' heel, i.e., the memory address space available to a given task was small compared with the data space accessed. There could be no solution to the problems using PDP-11 architecture. Having realized the limitations accentuated by our system, we found the DEC Virtual Address extension (VAX) series of computers suitable candidates for a migration path. With a large amount of main memory (about 2 Megabytes in the first system), extended sections of the most often used parts of the database remained in buffers, and rather than having to access the disk each time, a large proportion of requests resulted in immediate hits on data already in the buffers. The corresponding reduction in physical disk activity meant much faster operation of all tasks.

We decided to upgrade the PDP-11/60 to a VAX-11/750. To anticipate possible future performance limitations, however, we used as a benchmark a configuration identical with the one to be acquired. Two significant facts emerged from the exercise:

(1) the effort to convert the BASIC programs to run under the VAX-VMS operating system was small and

(2) the performance of the system vastly exceeded our expectations.

In fact, we were convinced that the maintenance and development team could share the machine unnoticed by the analysts in the lab.

In carrying out the benchmark, we had specified that a number of instrument communication lines be fed at the maximum sample rate at their respective data rates (4 lines at 1200 baud, samples on each at 10-second intervals and 8 lines at 300 baud, samples on each at 20-second intervals), thereby simulating 16 three-channel Technicon AutoAnalyzers and four AAs. In addition, two copies of our most demanding database applications and several other miscellaneous tasks were to be run simultaneously. The criterion for failure of the benchmark was the loss of any of the real-time data values on the instrument lines. The benchmark was set up and run for two hours, and no failure was encountered. To place an upper limit on the instrument loading for future reference in case of system expansion, we gradually increased the sampling baud rates on the data lines. The benchmark was eventually run at full speed on all data lines (12 lines solid data at 9600 baud) for 15 minutes without encountering any data losses. The system capacity was estimated at 15 to 20 times that of the PDP-11/60 for our application. We were convinced!

Slight modifications of the computer room were necessary to accommodate both the PDP-11/60 and the VAX-11/750 during the changeover. No problems were encountered with power consumption (the PDP 11/60 ran from its own three-phase, 208V line and the VAX ran on standard 110V, single phase) or with air conditioning load (the VAX produced less heat than the 11/60).

The current configuration of the VAX permits additional unplanned applications to run because of the excess capacity. Yet it is realized that due to operational considerations in the lab, these unplanned applications may have to be terminated or accommodated through a further upgrade to a larger machine.

In 1984, a considerable modification of the database structure was accomplished and the BASIC programs were modularized simultaneously. This was necessary to permit future changes to be introduced more simply. There are now 93 programs written in BASIC that are available to lab, supervisory and maintenance personnel.

CONCLUSION

We have succeeded in designing and developing an automated computerized data capture/management system for a modern well-equipped water chemistry analytical laboratory. During the eight-year period of system development, implementation and enhancement, we gained a considerable amount of experience from which, we believe, others could benefit. The system is now fully operational and, based on the results of a recent users' survey, seems to be meeting almost all of the laboratory's current needs. Given the dynamic nature of the laboratory operation, application demands on AWQUALABS vary with changing requirements. The flexible design of the system has permitted us to respond satisfactorily to these needs over the course of system development and implementation. We have had our share of problems during the development of the system, but working within a family of machines (PDP 11/34, 11/60 and VAX) having a simple and compatible upward migration path made possible our implementation of a progressively sophisticated application.

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